Theoretical Description of Ultrasonic Propagation and Scattering Phenomena in Polycrystalline Structures Aiming for Simulations on Nondestructive Materials Characterization and Defect Detection

Sigrun HIRSEKORN

Fraunhofer Institute for Nondestructive Testing (IZFP), Campus E3.1, 66123 Saarbrücken, Germany
Phone: +49 681 9302 3836, Fax: +49 681 9302 5903; e-mail: sigrun.hirsekorn@izfp.fraunhofer.de

Abstract
In microscopically inhomogeneous media ultrasonic scattering at grain and/or phase boundaries causes sound velocity dispersion and attenuation. These effects as well as the amplitudes of the scattering waves can be used for materials characterization. Concomitant, scattering at the microstructure of materials hampers defect detection and evaluation because the so-called structural noise superposes defect signals, and velocity dispersion corrupts defect positioning. Hence, the simulation of ultrasonic propagation and nondestructive testing procedures must contain microstructural scattering phenomena. In a general approach, the scattering wave energy flux densities in microscopically inhomogeneous materials are derived from the formal infinite Born series presentation of ultrasonic displacement vectors, the solutions of the elastodynamic equation of motion. The energy flux densities are ensemble averaged respective the microscopic inhomogeneity and evaluated for single phase polycrystals in lowest non-zero order. The resultant directional and frequency dependent scattering wave amplitudes are discussed in the context of results from the literature.

Keywords: microstructure, nondestructive testing, polycrystal, scattering, structural noise, theory, ultrasound

1. Introduction
The work presented here is carried out within the EC-FP7 Collaborative Project “Simulation Platform for Non-Destructive Evaluation of Structures and Materials (SIMPOSIUM)”. The objective of the ultrasonic part of SIMPOSIUM is the integration of scattering phenomena into the simulation of ultrasonic propagation and nondestructive testing and evaluation (ndt&e) experiments in microscopically inhomogeneous, e.g. polycrystalline, materials.

Scattering of ultrasound at microscopic inhomogeneities in materials, e.g. at grain boundaries in polycrystals, causes sound velocity dispersion and attenuation. These effects as well as the amplitudes of the scattered waves can be used for materials characterization. Concomitant, scattering at the microstructure of materials hampers defect detection and evaluation because the so-called structural or grain noise superposes the defect signals and velocity dispersion corrupts the exact defect positioning. This entails the need to include structural scattering into ultrasonic signal analysis and evaluation as well as nondestructive testing simulations.

In the late fifties, the attenuation of ultrasonic waves in polycrystalline materials due to grain scattering was determined using a single scatterer approach in first order Born approximation [1-2]. In the Rayleigh limit, i.e. for large wave length compared to the grain diameter, the far field approximation of the scattering waves and the ensemble average of their energy flux densities have been calculated. The ensemble average of a physical quantity is the statistical average concerning the microscopic inhomogeneity of a material in order to be reflective of its macroscopic behavior. In the following more than 50 years, comprehensive theoretical studies aiming for ensemble averaged intensities of scattering waves in microscopically inhomogeneous media arriving at transducers attached to sample surfaces for given incident waves have been carried out using the single scatterer approach or considerations based on the reciprocity theorem combined with the first order Born approximation (e.g. [3-15]).
In a more general approach the ensemble averaged elastodynamic equation of motion of a microscopically inhomogeneous material was solved [16-21] in second order Born [9-10, 12-20] and also Keller approximation [18, 21] (mathematical basics in [22]) in order to calculate sound velocity dispersion and attenuation due to ultrasonic scattering. The second order approximation was chosen because it yields the contribution of lowest order in the microscopic inhomogeneity if single phase polycrystalline materials, in which the linear part of the ensemble average is zero, are considered. The attenuation coefficients due to scattering obtained in [16-17] yield in the analytically determined Rayleigh limit the results of [1-2].

Numerical simulations of ultrasonic experiments require a convenient microstructural scattering model capable to simulate ultrasonic time signals, e.g. A-scans (backscattering signals), flexibility in shape and macroscopic material inhomogeneity (e.g. microstructure variations, defects, etc.) of the considered component, and analytical scattering coefficient formulae allowing fast simulation algorithms. Statistically distributed single scatterers the ensemble averaged scattering energy flux densities of which reflect the grain noise of the considered test block may be used as grain scattering model [23]. The convenient numerical simulation procedure is then point source synthesis of the scattering waves stemming from the scatterers mimicking structural noise and maybe also from defects including possible reflections at the sample surfaces. At the half space surface of a defect-free semi-infinite microscopically inhomogeneous solid of macroscopic homogeneity, the point source synthesis will yield the scattering wave intensities well-known from the literature [3-15].

The solutions of the general equation of motion of inhomogeneous materials contain not only the incident ultrasonic wave and its propagation behavior in the considered medium, but also the scattering waves, i.e. this approach may be exploited for scattering noise computations. In this work, the scattering wave energy flux densities in microscopically inhomogeneous materials are formally derived from the infinite Born series presentation of ultrasonic displacement vectors, the solutions of the elastodynamic equation of motion. The energy flux densities are ensemble averaged respective the microscopic inhomogeneity, evaluated for single phase polycrystals in lowest non-zero order and correlated to the model simulating grain scattering by statistically distributed single scatterers [23]. The resultant directional and frequency dependent scattering wave amplitudes are discussed in the context of well-known literature results. The numerical simulation procedure and ultrasonic propagation and ndt&e experiments in microscopically inhomogeneous media are correlated.

2. Elastodynamic equation of motion in case of microscopic inhomogeneity

The general equation of motion of a displacement vector \( s(r,t) \) in inhomogeneous materials

\[
\hat{L} s(r,t) = \sum_{j,k,l=1}^{3} \frac{\partial}{\partial x_j} \left( C_{jkl} \frac{\partial s^0_k(r,t)}{\partial x_l} \right) - \rho \frac{x^2}{\alpha^2} s(r,t) = 0, C_{jkl} = (C_{jkl}, C_{jkl}, C_{jkl}),
\]

contains position dependent second order elastic constants \( C_{jkl} = C_{jkl}(r) \) and density \( \rho = \rho(r) \) [e.g. 16-21]. The \( x_i \) are Cartesian coordinates. A virtual homogeneous material of position independent material constants is defined, the displacement vectors of which \( s^0(r,t) \) obey an equation of motion well adapted to the real material in order to be able to treat the microscopically inhomogeneous material, evaluated for single phase polycrystals in lowest non-zero order and correlated to the model simulating grain scattering by statistically distributed single scatterers [23]. The resultant directional and frequency dependent scattering wave amplitudes are discussed in the context of well-known literature results. The numerical simulation procedure and ultrasonic propagation and ndt&e experiments in microscopically inhomogeneous media are correlated.

Then, perturbation theory can be applied, and we obtain
The values in single phase polycrystal presentations of the grains. The density is constant, and the operator the orientation distribution function of the grains is constant averaged with the orientation distribution function of the grains as weighting factor anisotropy of the material, the position dependence of the grains and maybe also of secondary phase inclusions, as there are size, shape, and orientation distribution of the grains and maybe also of secondary microscopically, respectively

In the inhomogeneity, yields the Born approximation of nth order of the ultrasonic wave.

Generally, only statistical information about the microscopic inhomogeneity of the material, as there are size, shape, and orientation distribution of the grains and maybe also of secondary phase inclusions, is available via macroscopic material parameters. Thus, we have to aim for the ensemble average of the quantities, here marked by angled brackets. The ensemble averaged displacement vector \( s(r,t) \) in the material described by the operator \( \hat{L} \) (Eq. (1)) follows from Eq. (4c) and may be presented in two different ways:

\[
<s(r,t)> = \left\{ 1 - \hat{L}_0^{-1} \hat{A}_1 \right\}^{-1} s^0(r,t), \tag{5a}
\]

\[
\left\{ 1 - \hat{L}_0^{-1} \hat{A}_1 \right\}^{-1} <s(r,t)> = s^0(r,t). \tag{5b}
\]

Expansion up to second order in the small inhomogeneity \( \varepsilon \hat{L}_1 \) of Eqs. (5a) and (5b) yields the ultrasonic waves in the material in second order Born and in second order Keller approximation, respectively [16-21]. Both approximations are cut-off expansions with respect to the microscopic inhomogeneity of the material, which in single phase polycrystals is only caused by the single crystal anisotropy and the grain orientation, size, and shape distributions. Hence, the key parameter for weakness or strength of structural scattering is the single crystal anisotropy factor [16-21]. For low frequencies, i.e. in the Rayleigh regime and up to the resonance region, both approximations yield the same results. For higher frequencies (in the stochastic region and geometrical limit), differences become visible and the Born approximation is no longer valid [e.g. 18-20]. The Born approximation allows a straightforward computation, while the Keller approximation requires a self-consistent numerical evaluation of the analytical results. That is why in the following calculations the Born approximation is chosen.

3. Grain scattering in single phase polycrystalline materials

3.1 General formulae

In single phase polycrystalline materials, the density is constant, i.e. \( \rho'(r) \) in Eq. (3) is zero, and the position dependency of the elastic constants \( C_{ijkl}(r) \) is caused only by the single crystal anisotropy of the material and the different orientations of the grains. The values \( <C_{ijkl}(r)> \) averaged with the orientation distribution function of the grains as weighting factor may be chosen as elastic constants \( C_{ijkl}^0 \) of the virtual homogeneous material, and the linear term \( <\hat{A}_1> \) in the ensemble averaged equation of motion becomes zero. If no texture is present, the orientation distribution function of the grains is constant entailing macroscopic isotropy, and the operator \( \hat{A}^{-1}_1 \) and the inverse operator \( \hat{L}_0^{-1} \) are defined by Eqs. (5) and (7) in [21]:

\[
\hat{A}_1 u(r,t)=\sum_{j,k,l=1}^{3} \frac{\partial}{\partial x_j} \left( C_{ijkl}^0(r) \frac{\partial u_k(r,t)}{\partial x_l} \right) , \quad C^0_{ijkl}(r) = \left( C^0_{ijkl}(r), C^0_{jikl}(r), C^0_{ijkl}(r) \right) , \tag{6}
\]

\[
\hat{L}_0^{-1} u(r,t)=\sum_{j=1}^{3} \int d^3 r' G_j (r-r') u_j(r',t) , \quad G_j (r) = \left( G_{ji}(r), G_{j2}(r), G_{j3}(r) \right) , \tag{7}
\]

\[
G_{ij}(r)=-\frac{1}{r} \left[ \frac{x_i x_j}{r^2} g(r)+\delta_{ij} h(r) \right] , \quad \delta_{ij} = \begin{cases} 1 & \text{if } i = j , \\ 0 & \text{if } i \neq j \end{cases} , \quad G(r) = (G_{ij}(r)) , \tag{8a}
\]
\( g(r) = \frac{1}{4\pi \rho \omega^2 r^2} [3(1+ix) - x^2] e^{-ix|kr|}, \)  
\( h(r) = -\frac{1}{4\pi \rho \omega^2 r^2} [(1+ix)e^{-ikr} - (kr)^2 e^{-ikr}] . \)

\( u(r,t) \) is an arbitrary position and time dependent vector, \( G(r) \) is the Green’s function tensor in the monochromatic case:

\[ s(r,t) = s(r) e^{iat}, \quad s^0(r,t) = s^0(r) e^{iat}, \]

and \( \rho = \rho^0, k \) and \( \kappa \) are the wave numbers of compressional and shear waves, respectively, in the virtual homogeneous isotropic material. The wave numbers are related to the material properties via the wave lengths \( \lambda_L \) and \( \lambda_T \) and the sound velocities \( v_L \) and \( v_T \) of compressional and shear waves, respectively, by

\[ k = \frac{2\pi}{\lambda_L} = \frac{\omega}{v_L}, \quad \kappa = \frac{2\pi}{\lambda_T} = \frac{\omega}{v_T}; \quad \rho^0 v_L^2 = C_{11}^0, \quad \rho^0 v_T^2 = C_{44}^0 \]

and \( C_{11}^0 = C_{iiij}^0, \quad C_{12}^0 = C_{iiij}^0, \quad C_{44}^0 = C_{iiij}^0, \quad i,j = 1,2,3, i \neq j; \quad C_{11}^0 - C_{12}^0 - 2C_{44}^0 = 0. \)

The far field approximation of the Green’s function yields spherical waves:

\[ G_{ij}(r) = \sum_{r} \frac{x_i x_j}{r^2} g(r) + \delta_{ij} h(r) \to r \to \infty \]

\[ = -\frac{k^2}{4\pi \rho \omega^2} \frac{x_i x_j}{r^2} e^{-ikr} + \frac{k^2}{4\pi \rho \omega^2} \left( \frac{x_i x_j}{r^2} - \delta_{ij} \right) e^{-ikr}. \]

Ensemble averaged products of two elastic constants at positions \( r \) and \( r' \), respectively, are zero if both positions point into different grains. For \( r \) and \( r' \) pointing into the same grain, the results for hexagonal and cubic single crystal symmetry are given in [21]. The general representation of the ensemble averaged products is [18, 21]

\[ <C_{ijkl}(r)C_{mnp}(r')> = W(r-r') <C_{ijkl}^*C_{mnp}>, \]

with the ensemble average for \( C_{ijkl}^0 \) and \( C_{mnp} \) from the same grain

\[ <C_{ijkl}^0C_{mnp}^0> = <C_{ijkl}C_{mnp}^0> = <C_{ijkl}^0C_{mnp}>, \quad <C_{ijkl}^0> = C_{ijkl}, \]

and the probability that \( r \) and \( r' \) point into the same grain \( W(r-r') = \exp(-|r-r'|/\bar{d}), \) which is related to the effective grain volume by

\[ V_{\text{eff}} = \int d^3 r \ W(r) = 8\pi \bar{d}^3, \quad \bar{d} = 2 \ell, \]

\( \bar{d} \) is the mean free path length between two grain boundaries [18].

3.2. Ensemble averaged scattering wave intensities

The ensemble averaged scattering wave intensities are derived from complete solutions of the equation of motion in the polycrystalline material containing the incident and all scattering waves. This approach avoids excluding effects of close packed scatterers already at the starting point and ensures consistent abidance by the used approximations [e.g. 4, 5, 8, 9]:

- Born approximation (first order) of the ultrasonic waves, which implies weak and single scattering as well as validity limitation for large values of the wave number times grain diameter, i.e. limitation to the Rayleigh and resonance region.
- Far field approximation of the outgoing scattering waves (the distance of the point of observation to the origin of an outgoing scattering wave must be larger than the linear dimensions of the scattering volume) leading to outgoing spherical waves,
- The linear dimensions of the grains (about grain diameter in case of globular shape) have to be much smaller than the linear dimensions of the scattering volume (in order to fulfill the statistical conditions for ensemble averaging).

The intensity (or total energy flux) per unit area time averaged over one vibration cycle of a harmonic displacement field \( s(r,t) \) as given in Eq. (8d) is (* indicates conjugate-complex) [24]

\[ f_i(r) = \frac{\text{i} \omega}{4} \sum_{j=1}^{3} \left( \sigma_{ij}(r) s_j(r)^* - \sigma_{ij}(r)^* s_j(r) \right), \quad i = 1,2,3; \quad f(r) = (f_1(r),f_2(r),f_3(r)). \]
Hooke’s law relates the stress tensor \( \sigma_j(r) \) to the deformation tensor \( \varepsilon_{ij}(r) \) and the displacement vector \( s(r) \), and, exploiting the symmetry of the elastic constants \( C_{ijkl}(r) \), we obtain the position dependent total energy flux per unit area including its flow direction as

\[
f(r) = \frac{i\omega}{4} \sum_{j,k,l=1}^{3} C_{ijkl}(r) \left( \frac{\partial s_k(r)}{\partial x_l} - s_j(r) \frac{\partial s_k(r)}{\partial x_j} \right).
\]  

The Born series of a propagating wave, Eq. (4c), allows its presentation as infinite series in the microscopic inhomogeneity of the material:

\[
f(r) = \frac{i\omega}{4} \sum_{j,k,l=1}^{3} \left( C_{ijkl}^0 + C_{ijkl}(r) \right).
\]

\( f_n(r) \) is the term of nth order. The zeroth order term \( f^0(r) \) is the intensity of the incident plane wave \( s^0(r) \) (Eq. (8d)). It is explicitly evaluated for the wave \( s^0(r) = e_p \exp(-K r) \) with wave vector \( K = K e_K = K(n_{k1}, n_{k2}, n_{k3}) \) and polarisation \( e_p = (n_{p1}, n_{p2}, n_{p3}) \):

\[
f^0(r) = \frac{i\omega}{4} \sum_{j,k,l=1}^{3} C_{ijkl}^0 \left( \frac{\partial s_k^0(r)}{\partial x_l} - s_j^0(r) \frac{\partial s_k^0(r)}{\partial x_j} \right) = \frac{i\omega K}{2} \sum_{j,k,l=1}^{3} C_{ijkl}^0 n_{pj} n_{pk} n_{kl} = f^0.
\]

\( f^0 \) is innately independent of position and of the microscopic material inhomogeneity. The other terms of \( f(r) \) are due to the scattering waves. Following Eqs. (6) and (9), the zeroth order term (due to the incident wave) is not influenced by ensemble averaging of the total energy flux and the first order term becomes zero, \( <f^0(r)> = f^0, <f^1(r)> = 0 \). The second order part, \( <f^2(r)> \), is the one of lowest order in the microscopic inhomogeneity not equal to zero.

### 3.3. Ensemble averaged scattering wave energy flux densities and scattering coefficients

The ensemble averaged total energy flux due to scattering waves is the volume integral of the corresponding ensemble averaged energy flux density, \( <f^2_j(r'>) \) in 2nd order approximation,

\[
<f^2_j(r')> = <f^2> = \int d^3 r' <f^2_j(r')>.
\]

In case of macroscopic homogeneity, the ensemble averaged total energy flux has (and actually turned out) to be position independent. The integrand \( <f^2_j(r')> \) may represent the energy flux density of incoming or of outgoing waves respective to the origin of the coordinate system \( r' \). Because of the energy balance, the total energy flux of the incoming waves has to be equal to the total energy flux of the outgoing waves, i.e. Eq. (13) holds whatever waves the energy flux density, the integrand, represents, incoming or outgoing waves.

The ensemble averaged energy flux density of outgoing scattering waves \( <f^2_j(r'>) \) in the far field, i.e. for large \( r (r \to \infty) \), normalized with the energy flux per unit area of the incident wave (Eq. (12b)) provides with the scattering coefficient \( \eta_j^K(\partial, \phi, \omega) \) defined in [Eq. (1) of 9] (the upper index \( K = k, \kappa \) indicates the incident wave type, longitudinal and shear, respectively): \( \eta_j^K(\partial, \phi, \omega) d\Omega dV \) is the total power at angular frequency \( \omega \) scattered by grains within the volume \( dV \) into the solid angle \( d\Omega \) at direction \( (\partial, \phi) \) per unit incident sound intensity’:

\[
\eta_j^K(\partial, \phi, \omega) d\Omega dV = \int d\Omega' dV' <f^2_j(r'>).
\]
\[
\left( f^*(r) \cdot e_r \right) / (f^* \cdot e_k) \rightarrow_{r \rightarrow \infty} \frac{1}{r^2} \eta^K(\theta, \phi, \omega) = \frac{1}{r^2} \left( \eta^L_K(\theta, \phi, \omega) + \eta^T_K(\theta, \phi, \omega) \right).
\]

Here, \((r, \theta, \phi)\) are the spherical coordinates related to the Cartesian coordinate system \((x_1, x_2, x_3)\) by \(x_1 = r \sin \theta \cos \phi, x_2 = r \sin \theta \sin \phi, x_3 = r \cos \theta\), the origin of which is the centre of the scattering volume \(dV\), e.g. point \(P_1\) in Fig. 1; \(e_r\) (radial direction) and \(e_k\) are the propagation directions of the outgoing scattered and the incident wave, respectively. \(\eta^L_K(\theta, \phi, \omega)\) and \(\eta^T_K(\theta, \phi, \omega)\) are the coefficients for scattering into longitudinal and transverse waves, respectively. They are related to the far field amplitudes \(A^K_L(\theta, \phi, \omega)\) and \(A^K_T(\theta, \phi, \omega)\) of outgoing longitudinal and transverse spherical waves [Eq. (2) and Fig. 1 in 9] by

\[
\eta^K_{K_s}(\theta, \phi, \omega) = n < |A^K_{K_s}(\theta, \phi, \omega)|^2 > \frac{v_{K_s}}{v_K}, \quad K_s = L, T;
\]

\(n\) is the number of scatterers per volume, and \(v_{K_s}\) and \(v_K\) are the sound velocities of the scattered waves and the incident wave, respectively. As already pointed out, the origin of the outgoing scattered waves is the centre of a scattering volume \(dV\), e.g. point \(P_1\) in Fig. 1, and, following the definitions in the right hand side of Fig. 1 in [9], the far field ultrasonic scattering coefficients \(\eta^K_L(\theta, \phi, \omega)\) and \(\eta^K_T(\theta, \phi, \omega)\) and amplitudes \(A^K_L(\theta, \phi, \omega)\) and \(A^K_T(\theta, \phi, \omega)\) are presented in a coordinate system with its origin there. The definitions of \(\eta^K_{K_s}(\theta, \phi, \omega)\) and \(A^K_{K_s}(\theta, \phi, \omega)\) are chosen analogously to those for single inclusions in a homogeneous material matrix [e.g. 24].

Figure 1. Incident plane wave (wave vector \(K\)) propagating into the positive \(x_1\)-direction being scattered at statistically distributed scatterers in the sample; the figures show the \(x_1-x_2\)-plane, the \(x_2\)-direction is perpendicular to it as indicated in the small side pictures: a) spherical scattering waves outgoing from a scatterer (or scattering volume \(dV\)) e.g. at position \(P_1\) (scattering wave vector \(K_s\), propagation into the positive \(e_r\)-direction); b) spherical scattering waves incoming e.g. to the position \(P_2\) (wave vector \(K_s\), propagation into the negative \(e_r\)-direction).

Grain noise simulations, i.e. the simulation of scattered time signals as e.g. A-scans (backscattering time signals), require the directional characteristics of the scattered waves outgoing from the scattering volume elements \(dV\) as defined by Eq. (14a) and verbally in Eq. (1) of [9]. Calculations aiming for the directional characteristic of the power of scattering waves incident onto an ultrasonic receiver probe at the sample surface (e.g. at \(P_2\) in Fig. 1) may be carried out via the energy flux density of incoming waves respective to a coordinate system with its origin at \(P_2\) delivering the total power of all scattering waves incoming into a solid angle \(d\Omega\) at a direction \((\theta, \phi)\) of a coordinate system the origin of which is at \(P_2\). The energy flux density of incoming waves is the superposition of scattering waves stemming from all scatterers in the medium which reach this point, i.e. the phase information of individual scatterers is lost in the results, and thus, they cannot be used for scattering time signal simulations requiring phase dependent constructive and destructive superposition of the scattering waves.
The normalized ensemble averaged energy flux density (Eq. (14a)) is analytically evaluated using the approximations listed above. It turned out that the far field approximation \( (r \to \infty) \) of Eq. (14a) with \( 1/r^2 \) dependency on distance \( r \) only contains scattering waves of single scatterers in first order Born approximation. All other contributions fall off faster with increasing \( r \).

As suggested in [1] and already pointed out above, the difference between incoming and outgoing waves has to be considered carefully. The ensemble averaged energy flux density used for the evaluation of Eq. (14a) in order to determine the scattering coefficients \( \eta_f(\vartheta, \varphi, \omega) \) has to be that one of outgoing waves. The sign of \( \langle \hat{f}_i(r) \cdot \hat{e}_r \rangle / \langle \hat{f}_o \cdot \hat{e}_K \rangle \) in the far field, which reflects the flow direction of the scattered intensity in relation to the flow direction of the incident intensity, is the identifying feature. In the far field, outgoing waves propagate into the positive \( e_r \)-direction, i.e. \( \langle \hat{f}_i(r) \cdot \hat{e}_r \rangle \) has to be positive. For an incident plane wave propagating into the positive \( e_x \)-direction \( (e_K = e_x) \), \( \langle \hat{f}_o \cdot \hat{e}_K \rangle \) is positive (Eq. (12b)). Then, the sign of \( \langle \hat{f}_i(r) \cdot \hat{e}_r \rangle / \langle \hat{f}_o \cdot \hat{e}_K \rangle \) must be positive for outgoing scattering waves, the wave vector of which is \( K_s = K_x e_x \). The spherical and Cartesian coordinates (see above) yield backscattering, i.e. scattering waves propagating into \(-e_r\)-direction, for the radial unit vector \( e_r \), with \( \vartheta = \pi \).

For an incident plane longitudinal wave

\[
\mathbf{s}^0 (r) = e_p \, e^{iK \cdot r}, \quad \mathbf{K} = ke_K, \quad e_K = (n_{K1}, n_{K2}, n_{K3}), \quad e_p = (n_{p1}, n_{p2}, n_{p3}),
\]

(15a)

propagating into the positive \( e_x \)-direction, i.e. \( n_{pj} = n_{Kj} = 1 \) if \( j = 3 \), \( n_{pj} = n_{Kj} = 0 \) if \( j = 1, 2 \), we obtain

\[
\eta_f^L(\vartheta, \varphi, \omega) = \frac{k^8 \omega^3 \pi}{(4\pi \rho_0)^2} \left\{ 1 + k^2(1 + \cos \vartheta) \frac{d^2}{2} \right\}^2 \cdot \begin{cases}
(C_{3333}^2 > \cos^4 \vartheta + (C_{1133}^2 > \sin^4 \vartheta + 2(C_{1133}^2 + 2(C_{1133}^2 > \sin^2 \vartheta \cos^2 \vartheta)), \\
(C_{1233}^2 > \sin^2 \vartheta + (C_{1133}^2 > + 2(C_{1133}^2 > - 2(C_{1133}^2 > - 4(C_{1133}^2 > \sin^2 \vartheta \cos^2 \vartheta)).
\end{cases}
\]

(15b)

The type of the incident and of the scattered wave is indicated by the upper and the lower index, respectively, \( d \) is the mean free path length between grain boundaries (Eqs. (9)).

Analogously, for an incident plane shear wave

\[
\mathbf{s}^0 (r) = e_p \, e^{iK \cdot r}, \quad \mathbf{K} = ke_K, \quad e_K = (n_{K1}, n_{K2}, n_{K3}), \quad e_p = (n_{p1}, n_{p2}, n_{p3}),
\]

(16a)

with propagation into the positive \( e_x \)- and polarization into \( e_1 \)-direction, i.e. \( n_{Kj} = 1 \) if \( j = 3 \), \( n_{Kj} = 0 \) if \( j = 1, 2 \), \( n_{pj} = 1 \) if \( j = 1, 2 \), \( n_{pj} = 0 \) if \( j = 2, 3 \), we obtain the scattering coefficients

\[
\eta_f^T(\vartheta, \varphi, \omega) = \frac{k^8 \omega^3 \pi}{(4\pi \rho_0)^2} \left\{ 1 + (k^2 + \kappa^2 + 2k \cos \vartheta) \frac{d^2}{4} \right\}^2 \cdot \begin{cases}
(C_{2213}^2 > \sin^4 \theta \cos^4 \theta + \cos^4 \theta + 2(C_{1113}^2 > + 2(C_{1113}^2 > \sin^2 \theta \cos^2 \theta \cos^2 \varphi) + 2(C_{1113}^2 > + 2(C_{1113}^2 > \sin^2 \theta \sin^2 \varphi (\sin^2 \theta \cos^2 \theta \cos^2 \varphi)), \\
(C_{1113}^2 > + (C_{2213}^2 > - (C_{1113}^2 > - 4(C_{1113}^2 > \sin^2 \theta \sin^2 \varphi (\sin^2 \theta \cos^2 \theta \cos^2 \varphi)).
\end{cases}
\]

(16b)
Calculations for an incident plane shear wave with propagation into positive $e_3$- and polarisation into $e_2$-direction yield the same results, but with exchanged indices 1 and 2. The ensemble averaged values of the elastic constants $<C_{ijkl}>$ and of their products $<C_{ijkl}C_{mnop}>$ for isotropic orientation distribution of the grains (macroscopic isotropy) and cubic as well as hexagonal single crystal symmetry can be found in the literature [e.g. 21].

The analogue analytical evaluation of the equation for incoming waves (equivalent to Eq. (14a)) yields the results given in [9]. Thus, the directional characteristic of the scattering coefficient $\eta_L(\vartheta,\phi,\omega)$ describing an incident longitudinal wave being scattered into outgoing longitudinal waves (Eq. (15b)) is identical with the analytical result for incoming longitudinal scattering waves [9] in which the sign of the scattering wave vector is changed ($-K_S$ replaced by $K_S$) due to the energy flow direction of incoming waves. In contrary to [9], the calculations presented here do not explicitly distinguish between shear horizontal and shear vertical waves because this definition is fixed to a sample surface. Because of symmetry reasons, the polarization of outgoing spherical scattered shear waves will be $e_\varphi=(\cos \vartheta \cos \varphi, \cos \vartheta \sin \varphi, -\sin \vartheta)$ in the scatterer fixed spherical coordinate system. The numerical evaluation of Eqs. (15) and (16) for one example of [9] using exactly the same data as given there (including the replacement of the mean free path length between two grain boundaries $\bar{d}$ by the grain diameter in the analytical formulae) yields Fig. 2. As pointed out above, the scattering coefficient $\eta_L(\vartheta,\phi,\omega)$ shows the mirrored directional characteristic of the corresponding incoming spherical wave.

4. Conclusion

Grain noise may be simulated by statistically distributed scatterers in a medium [23]. Their directional dependent scattering amplitudes are determined from the ensemble average of the energy flux densities of the scattering waves (Eqs. (14), (15), and (16)). The ultrasonic time signals are then computed by point source synthesis, i.e. at a chosen position (e.g. ultrasonic receiver attached to a sample surface) all scattering waves are superposed taking into account their relative phases. The result is observed as function of time. Numerical simulations using statistical scatterer distributions will never reproduce an actually measured ultrasonic time signal, but will yield signals which a virtual sample with the same macroscopic behavior as the real sample under consideration might generate. Simulated ultrasonic time signals reflect the interference pattern of the statistical distribution of the scatterers involved, while meas-
ured A-scans reflect the interference pattern of the special grain arrangement along the sound path comprising orientation, shape, and size of each grain.

Experimental ensemble averaging may be performed by appropriate averaging of congeneric A-scans of different sound paths. At first view, small variations in probe position on the surface of a polycrystalline sample will result in completely different A-scans [e.g. 25]. The statistical distribution of the grain boundaries leads to phase shifts in the result of the sum of all scattering signals which contribute to a fixed time of flight in a fixed sound path. As a consequence, averaging of different measured congeneric A-scans reduces the grain noise significantly. This effect might be exploited for contrast enhancement in ultrasonic defect detection, but will work only very limited because the signal averaging will reduce the defect signal as well, at least for oblique sound incidence onto the surface of the defect. In order to obtain ensemble averaged backscattering amplitudes of the material, position averaging of rectified measured A-scans was proposed [25]. The exponential decay of averaged rectified A-scans yields the ultrasonic attenuation coefficient due to scattering, and a signal to noise ratio enhancement is achieved for defects comparable to grain size or larger. When comparing with theory, one has to keep in mind that experimental position averaging cannot comprise full ensemble averaging as long as a reasonable spatial resolution shall be kept. The numerical procedure using point source synthesis of statistically distributed scatterers for structural noise simulations as described above contains the capability to simulate also the experimental way of ensemble averaging of ultrasonic time signals. Furthermore, point sources describing defects and possible reflections at complicated sample surfaces can easily be introduced.

Even though grain noise simulations based on calculated ultrasonic scattering energy flux densities and statistical scatterer distributions will never reproduce actually measured ultrasonic time signals, the numerical procedure is very useful to demonstrate complicated ultrasonic testing tasks and illustrate possibly arising problems. Additionally, it may point out promising testing scenarios. The simulations may decide about the practicability of techniques when applied to complex components composed of microscopically inhomogeneous media and may support nondestructive testing friendly design of components. The provided analytical fundamentals allow fast simulations of complicated ultrasonic ndt&e experiments. The underlying general mathematical formalism enables the extension of the theory to multi-phase and macroscopically anisotropic and inhomogeneous materials. The far field approximation of the scattering waves might be dropped. Higher expansion terms might be considered in order to allow strong and multiple scattering and the investigation of close packed scatterer effects.

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